CPT-Invariant Eight-Component Two-Fermion Equation

Viktor Hund

Institut für Theoretische Teilchenphysik, Universität Fridericiana, D-76128 Karlsruhe, Germany

Abstract. A Dirac equation with hyperfine operator and a recoil structure that remains valid even for positronium is presented and applied to the muonium hyperfine structure to the ordern α^8.

1 Introduction

When describing arbitrary two-body systems fully relativistically, one would expect that the formalism produces explicitly $\mathcal{CPT}$-invariant results. $\mathcal{CPT}$-invariance requires symmetry of the terms under change of the sign of the system's total energy $E_1 + E_2 = E \longleftrightarrow -E$, also for bound states where the individual energies E_1 and E_2 are not conserved. This means that the decisive equations should contain only even powers of E.

The standard approaches for two-fermion systems like Bethe-Salpeter or Dirac-Breit satisfy this condition. But usually this property is lost in the final results, because (nonrelativistic) approximations (e.g. $E_i \approx m_i$) are used for one or both particles to simplify the calculation.

In the following, an approach is presented that reproduces the main part of the recoil and hyperfine corrections without any nonrelativistic approximation and therefore with full $\mathcal{CPT}$-invariance.

In sections 2 and 3, the derivation of the free equation and the implementation of the interaction in it is briefly outlined. The main point of this approach is that equation and wave function, in which the interaction has to be inserted, have only 8 components instead of 16. This means that an irreducible representation for a two-fermion system is used ($2_{spin1} \otimes 2_{spin2} \otimes 2_{parity}$ instead of $4 \otimes 4$).

In section 4, the perturbation scheme is presented and the results are checked against current NRQED calculations [1] up to the order α^6.

Section 5 gives some concluding remarks.

2 The free eight-component two-fermion equation

Starting point are the Dirac equations of the two particles ($i = 1, 2$) [2]. At this point of the calculation with external potentials $A_i^\mu(\boldsymbol{r}_i) = (V_i/q_i, \boldsymbol{A}_i)$, $\pi_i^\mu = p_i^\mu + A_i^\mu$ ($p_i^\mu = (\mathrm{i}\partial_t, -\mathrm{i}\nabla)$, $\hbar = c = 1$), which is more general than [2].

$$\mathcal{K}_{Di}\psi_i = [\gamma_i^\mu \pi_{i\mu} - m_i]\psi_i = 0 = [\pi_i^0 - m_i\gamma_i^0 - \gamma_i^5 \boldsymbol{\sigma}_i \boldsymbol{\pi}_i]\psi_i$$

with the standard definitions for the Dirac matrices $\gamma_i^\mu = (\gamma_i^0, \gamma_i^0\gamma_i^5\boldsymbol{\sigma}_i)$. Addition of the two Dirac equations gives a 16-component form of the equation for this system:

$$\left[\pi_1^0 + \pi_2^0 - m_1\gamma_1^0 - m_2\gamma_2^0 - \gamma_1^5\boldsymbol{\sigma}_1\boldsymbol{\pi}_1 - \gamma_2^5\boldsymbol{\sigma}_2\boldsymbol{\pi}_2\right] \Psi^{(16)} = 0 \ .$$

Here the asumption is $\mathcal{K}_{Di}\Psi^{(16)} = 0$ as in the potential-free case ($A_i^\mu = 0$), where $\Psi^{(16)} = \psi_1 \otimes \psi_2$.

The 16-component wave function is now divided into two 8-component parts $\Psi^{(16)} = (\psi, \chi)$, which have the following properties:

$$\gamma_1^5 \begin{pmatrix}\psi\\ \chi\end{pmatrix} = \begin{pmatrix}\gamma^5\psi\\ \gamma^5\chi\end{pmatrix},\ \gamma_2^5 \begin{pmatrix}\psi\\ \chi\end{pmatrix} = \begin{pmatrix}\gamma^5\psi\\ -\gamma^5\chi\end{pmatrix},\ \gamma_1^0 \begin{pmatrix}\psi\\ \chi\end{pmatrix} = \begin{pmatrix}\gamma^0\chi\\ \gamma^0\psi\end{pmatrix},\ \gamma_2^0 \begin{pmatrix}\psi\\ \chi\end{pmatrix} = \begin{pmatrix}\chi\\ \psi\end{pmatrix} .$$

γ^5 and γ^0 act on the components of ψ and χ like the operators in the one-particle case, especially $\{\gamma^5, \gamma^0\} = 0$ and ${\gamma^5}^2 = 1 = {\gamma^0}^2$.

The 16-component equation becomes a system of two coupled equations

$$\begin{aligned}(m_2 + m_1\gamma^0)\chi &= \left[\pi^0 - \gamma^5(\boldsymbol{\sigma}_1\boldsymbol{\pi}_1 + \boldsymbol{\sigma}_2\boldsymbol{\pi}_2)\right]\psi \equiv \left[\pi^0 - \gamma^5\pi_+\right]\psi \\ (m_2 + m_1\gamma^0)\psi &= \left[\pi^0 - \gamma^5(\boldsymbol{\sigma}_1\boldsymbol{\pi}_1 - \boldsymbol{\sigma}_2\boldsymbol{\pi}_2)\right]\chi \equiv \left[\pi^0 - \gamma^5\pi_-\right]\chi \end{aligned} \qquad (1)$$

with $\pi^0 = \pi_1^0 + \pi_2^0$. Elimination of the χ-components produces an 8-component equation. After multiplication with $m_2 + m_1\gamma^0$ it reads

$$\left[{\pi^0}^2 - (m_2 + m_1\gamma^0)^2 + \pi_-\pi_+\mu_\gamma - \gamma^5\left(\pi^0\pi_+ + \pi_-\pi^0\frac{1}{\mu_\gamma}\right)\right]\psi = 0 \qquad (2)$$

with $\mu_\gamma = (m_2 + m_1\gamma^0)/(m_2 - m_1\gamma^0) = (m_2 + m_1\gamma^0)^2/(m_2^2 - m_1^2)$.

The terms containing μ_γ seem to be problematic in the case of equal masses ($m_1 = m_2$) – but they are not. A second reduction of the number of components to 4 shows that all divergent terms cancel. If the external potentials are neglected ($A_i^\mu = 0$), the disturbing mass-factors may be eliminated in the above 8-component form in the center-of-mass-system (cms) [2], where $\boldsymbol{p}_1 = \boldsymbol{p} = -\boldsymbol{p}_2$ implies

$$\pi_-\pi_+ = (\boldsymbol{\sigma}_1\boldsymbol{p}_1)^2 - (\boldsymbol{\sigma}_2\boldsymbol{p}_2)^2 = 0$$

which means that the equation is linear in $\boldsymbol{p}$:

$$\left[E^2 - (m_2 + m_1\gamma^0)^2 - \gamma^5 E\left(\boldsymbol{p}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2) + \boldsymbol{p}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\frac{1}{\mu_\gamma}\right)\right]\psi = 0$$

with the cms-energy $\sqrt{s} = E = \pi^0 = E_1 + E_2$ in that case.

The factor $1/\mu_\gamma$ can be removed by a transformation of the wave function which fulfills the following conditions:

$$\psi = c\psi_c, \quad \bar{c}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)c \stackrel{!}{=} (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2), \quad \bar{c}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)c \stackrel{!}{=} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\mu_\gamma\ .$$

$\bar{c}$ occurs when the equation is multiplied by $1/c$ from left, $c^{-1}\gamma^5 = \gamma^5\bar{c}$. For the c found is $\bar{c} = c$:

$$c = (m_2^2 - m_1^2)^{-1/2}[m_2 + \gamma^0 m_1\frac{1}{2}(1 + \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)]\ . \tag{3}$$

It must be emphasized that this transformation is not unique. One can impose for example $\bar{c}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)c \stackrel{!}{=} -(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)$ or $\bar{c}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)c \stackrel{!}{=} (\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)/\mu_\gamma$, $\bar{c}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)c \stackrel{!}{=} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)$ and then ends at slightly modified transformations.

The result is always an equation linear in $\boldsymbol{p}$ with just one set of Pauli matrices $\boldsymbol{\sigma}_1$ or $\boldsymbol{\sigma}_2$; with the transformation (3), $\boldsymbol{\sigma}_1$ appears in

$$\left[E^2 - m_2^2 - m_1^2 - 2m_2m_1\gamma^0 - 2\gamma^5 E\boldsymbol{p}\boldsymbol{\sigma}_1\right]\psi_c = 0$$

or, using a relativistic reduced mass $\mu = m_2m_1/E$ and reduced energy $\varepsilon = (E^2 - m_2^2 - m_1^2)/2E$ to get a dimensionless form in a variable ϱ:

$$\left[\frac{\varepsilon}{\mu} - \gamma^0 - \gamma^5\boldsymbol{p}_\varrho\boldsymbol{\sigma}_1\right]\psi_c = 0, \qquad \boldsymbol{\varrho} = \mu\boldsymbol{r}, \quad \boldsymbol{p}_\varrho = \frac{\boldsymbol{p}}{\mu}\ . \tag{4}$$

3 Introduction of the interaction in the 8-component equation

Here, the S-matrix is also used for the interaction between the two particles. The Fourier-transform of the first Born approximation produces the potential in the 8-component equation.

In first Born approximation, the wave function is the product of a plane wave and a part which contains only the spin structure ($\psi = u\mathrm{e}^{\mathrm{i}\phi}$, $\phi = -K^\mu x_\mu = \boldsymbol{KR} - Et$). Integration over d^4x generates the energy and momentum conserving δ-functions, which are explicitly removed in the definiton of the T-matrix. The main point is now the connection between the 16×16 $T_{if} = \bar{u}_1'\bar{u}_2'\hat{T}u_1u_2$ and its 8×8 form M. Defining in analogy to the one-particle case

$$\Psi^{(16)}(x) = \begin{pmatrix} \psi \\ \chi \end{pmatrix} = \begin{pmatrix} v \\ w \end{pmatrix} \mathrm{e}^{\mathrm{i}\phi}, \quad \phi = \phi_1 + \phi_2 = -K_1^\mu x_{1\mu} - K_2^\mu x_{2\mu}$$

one can transform $u_1u_2 \longleftrightarrow v, w$ (primed expressions analogous):

$$T_{if} = \bar{u}_1'\bar{u}_2'\hat{T}u_1u_2 = v'^\dagger T_v v + v'^\dagger T_{vw} w + w'^\dagger T_{wv} v + w'^\dagger T_w w$$

For the first Born approximation of T_{if}, $T_{vw} = 0 = T_{wv}$ is found.

T_{if} may be brought into the form

$$T_{if} = w'^\dagger M v \quad \text{or} \quad T_{if} = v'^\dagger M_\chi w \quad \text{with} \quad M = M_\chi^\dagger \tag{5}$$

depending on the equation for which the interaction is constructed [3] (the left T_{if} is used for the ψ-equation, the right one for χ).

One may compare this property with the one-particle case, where a different interaction arises in the 2-component Kramers-form of the Dirac equation for big and small components.

The form (5) can be achieved using the coupled equations (1) for w and v. After the c-transformation (3) of v (and with the appropriate c_χ for w), with $A_i^\mu = 0$ in the cms T_{if} becomes

$$T_{if} = w_c'^\dagger \left[(E' - \gamma^5 \boldsymbol{k}'(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)) \frac{1}{c} T_v c + c_\chi^\dagger T_w \frac{1}{c_\chi^\dagger} (E - \gamma^5 \boldsymbol{k}(\boldsymbol{\sigma}_1 - \boldsymbol{\sigma}_2)) \right] v_c \,.$$

For the well-known first Born approximation $T_{if} = \alpha\bar{u}_1'\bar{u}_2'(\gamma_1^\mu\gamma_{2\mu}/q^2)u_1u_2$, the resulting interaction potential (for elastic scattering $q^0 = E - E' = 0$) in the dimensionless equation (4) is [4]

$$V_\psi(\varrho) = V_C - \mathrm{i}\gamma^5 \frac{m_1m_2}{E^2} V_C (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2)\boldsymbol{p}_\varrho, \qquad V_C = -\frac{\alpha}{\varrho}$$

It is the sum of the ordinary Coulomb potential and a hyperfine operator.

4 Perturbation theory and results

As usual, the dimensionless equation with interaction is separated in an exactly solvable part containing the Coulomb potential V_C and a perturbation W_P

$$\left[\frac{\varepsilon}{\mu} \underbrace{-\gamma^0 - V_C - \gamma^5 \boldsymbol{p}_\varrho \boldsymbol{\sigma}_1}_{-H_0} \underbrace{+\mathrm{i}\gamma^5 \frac{m_1 m_2}{E^2} V_C (\boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2) \boldsymbol{p}_\varrho}_{-W_P}\right] \psi_c = 0\,. \tag{6}$$

The results of the exact equation $(\varepsilon/\mu)^{(0)} \psi_c^{(0)} = H_0 \psi_c^{(0)}$ are well-known from the ordinary Dirac equation; replacing $E, m \to \varepsilon, \mu$ results in [2, 4]:

$$\frac{\varepsilon}{\mu} = f_D = \sqrt{\left(1 + \frac{\alpha^2}{{n_D^*}^2}\right)^{-1}}\,, \quad n_D^* = n + \gamma - j - \frac{1}{2}$$

(n = principal quantum number, $j = \ell + s_1$ = total angular momentum of particle 1, $\gamma = \sqrt{(j+1/2)^2 - \alpha^2}$).

As $\varepsilon/\mu = (E^2 - m_1^2 - m_2^2)/2m_1 m_2$, this result is $\mathcal{CPT}$-invariant. For a check using the present NRQED results, it is necessary to caculate $E - m$ instead of $E^2 - m^2$ ($m = m_1 + m_2$ being the total mass):

$$E - m = m\sqrt{1 + 2\frac{\mu_{nr}}{m}(f_D - 1)} - m = \mu_{nr}(f_D - 1) - \frac{\mu_{nr}^2}{2m}(f_D - 1)^2 + \ldots$$

with $\mu_{nr} = m_1 m_2/m$ and the above f_D. This could be expanded in arbitrary orders in α.

The perturbation theory is performed in the usual way, but for ε/μ which is $E^2/2m_1 m_2$. This means that any shift $\delta(\varepsilon/\mu)$ corresponds to a shift δE:

$$\delta(\varepsilon/\mu) = \delta(E^2/2m_1 m_2) = \frac{E}{m_1 m_2}\delta E = \frac{1}{\mu}\delta E\,. \tag{7}$$

So the first-order shift caused by the hyperfine operator W_P contributes to $E^{(1)}$ [4]:

$$E_{hf}^{(1)} = \mu\left(\frac{\varepsilon}{\mu}\right)_{hf}^{(1)} = \alpha^4 \frac{\mu^2}{E} \frac{4(f-j)}{f+1/2} f_D^3 \frac{(j+1/2)^2 f_D - \kappa_D/2}{n_D^{*3} \gamma (2\gamma+1)(2\gamma-1)} \tag{8}$$

$f = j \pm 1/2$ is the total angular momentum, and $\kappa_D = 2(\ell - j)(j + 1/2)$. For E (and also in $\mu^2 = m_1^2 m_2^2/E^2$), the unperturbed value $E^{(0)}$ will be used. (8) applies for arbitrary states.

For the nS-states (i.e. $j = 1/2$), $E_{hf}^{(1)}$ will be given to the order α^8:

$$E_{hf}^{(1)} \approx \frac{\mu_{nr}^2}{m} \alpha^4 f_{hf,D}^{(1)} \left[1 + 3\frac{\mu_{nr}}{m}\frac{\alpha^2}{2n^2}\left(1 - \frac{3}{4}\frac{\alpha^2}{n^2} + \frac{\alpha^2}{n}\right)\right]$$

with

$$f^{(1)}_{hf,D} = \frac{4(f-j)}{(2f+1)n^3}\,(1+\alpha^2 c_2 + \alpha^4 c_4),$$

$$c_2 = \frac{11}{6} + \frac{3}{2n} - \frac{11}{6n^2}, \qquad c_4 = \frac{1}{4}\left(\frac{203}{18} + \frac{25}{2n} - \frac{67}{9n^2} - \frac{55}{3n^3} + \frac{21}{2n^4}\right)\,.$$

This is the $\mathcal{CPT}$-invariant result from the one-photon exchange potential. To order α^6, it comprises all terms found by Pachucki [1] except for $\alpha^6 \log\alpha$ and n-independent terms. (Among these are on the one hand the hyperfine mixing of states with equal total angular momentum f and different $j = \ell + s_1$ (for example the S-D-mixing) and on the other hand contributions of higher-order graphs. First higher-order effects arise at the order α^5/π and are caused by two-photon exchange.)

The structure of the leading α^8-term ($\sim \alpha^8 \mu_{nr}^2/m$) was assumed by Kinoshita [5]; all further α^8-results are new and need confirmation by other calculations.

5 Concluding remarks

Although the 8-component equation given in (6) looks unusual in its asymmetry between the two particles, the comparison with NRQED results shows its correctness.

The following points make this formalism interesting:

- The dimensionless equation (6) is explicit $\mathcal{CPT}$-invariant.
- The formalism has 8 components and is therefore an irreducible representation of the Lorentz group. This implies that
  - the interaction generated by the scattering matrix is non-hermitian (to compare to the Dirac equation in irreducible Kramers-form with 2 components).
  - the first order interaction includes the main part of the interaction normally attributed to two-photon exchange, namely $-V^2$ (The 16-component interaction $(E-V)$ becomes $(E-V)^2$ in 8 components, and $(E-V)^2 - V^2 = E^2 - 2EV = E^2 - 2m_1m_2V_\varrho$ gives already the 8-component first order potential V_ϱ).
- In the cms, the equation is linear in the momentum $\boldsymbol{p}$.
- The "Dirac-Coulomb-equation" (i.e. the dimensionless equation with Coulomb potential) has exact solutions and can therefore be used as a good starting point for perturbation theory.

References

1. K. Pachucki: Phys. Rev. A **56**, 297 (1997); Phys. Rev. Lett. **79**, 4120 (1997)
2. R. Häckl, V. Hund, H. Pilkuhn: Phys. Rev. A **57**, 3268 (1998); **60**, 725E (1999)
3. V. Hund: *Empirische Gleichungen für relativistische Zweiteilchensysteme.* Ph.D. Thesis, Universität Karlsruhe (Shaker Verlag, Aachen 1998)
4. V. Hund, H. Pilkuhn: J. Phys. B **33**, 1617 (2000)
5. T. Kinoshita: preprint hep-ph/9808351 (1998)
6. M. Malvetti, H. Pilkuhn: Phys. Rep. C **248**, 1 (1994)